Acta Crystallographica Section E

Structure Reports Online

ISSN 1600-5368

2-Naphthyl quinoxalin-2-yl ether

Noor Doha Hassan, Hairul Anuar Tajuddin, Zanariah Abdullah and Seik Weng Ng*

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

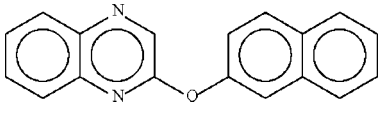
Received 2 March 2009; accepted 4 March 2009

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.048; wR factor = 0.127; data-to-parameter ratio = 16.3.

In the crystal structure of the title compound, $C_{18}H_{12}N_2O$, the two fused rings are aligned at 64.2 (1)°; the C—O—C angle is 118.73 (12)°.

Related literature

For the crystal structure of 1-naphthyl quinoxalinyl ether, see: Hassan *et al.* (2009).



Experimental

Crystal data

$C_{18}H_{12}N_2O$ M_r = 272.30
Monoclinic, $P2_1/c$
a = 6.808 (1) Å
b = 7.609 (1) Å
c = 26.234 (3) Å
β = 92.522 (2)°
V = 1357.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 K
0.45 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
7510 measured reflections
3094 independent reflections
1950 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.127
S = 1.04
3094 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank the University of Malaya for supporting this study (FS358/2008 A).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2387).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Hassan, N. D., Tajuddin, H. A., Abdullah, Z. & Ng, S. W. (2009). *Acta Cryst.* E**65**, o731.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2009). *publCIF*. In preparation.

supplementary materials

Acta Cryst. (2009). E**65**, o732 [**doi:10.1107/S1600536809007855**]

2-Naphthyl quinoxalin-2-yl ether

N. D. Hassan, H. A. Tajuddin, Z. Abdullah and S. W. Ng

Comment

(type here to add)

Experimental

2-Naphthol (2.88 g, 20 mmol) was mixed with sodium hydroxide (0.08 g, 20 mmol) in several drops of water. The water was then evaporated. The paste was heated with 2-chloroquinoxaline (3.29 g, 20 mmol) at 423–433 K for 6 h. The product was dissolved in water and the solution extracted with chloroform. The chloroform phase was dried over sodium sulfate; the evaporation of the solvent gave a product that was recrystallized from an ethyl acetate/hexane.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C).

Figures

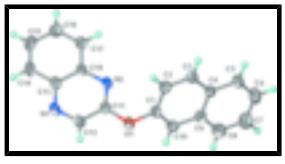


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of the molecule of $C_{18}H_{12}N_2O$ at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

2-Naphthyl quinoxalin-2-yl ether

Crystal data

$C_{18}H_{12}N_2O$	F_{000} = 568
M_r = 272.30	D_x = 1.332 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1541 reflections
a = 6.808 (1) Å	θ = 2.7–28.2º
b = 7.609 (1) Å	μ = 0.08 mm^{-1}
c = 26.234 (3) Å	T = 295 K
β = 92.522 (2)º	Block, colorless
V = 1357.5 (3) Å^3	0.45 × 0.15 × 0.10 mm
Z = 4	

Data collection

Bruker SMART APEX diffractometer	1950 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.032$
Monochromator: graphite	$\theta_{max} = 27.5^{o}$
$T = 295$ K	$\theta_{min} = 2.8^{o}$
ω scans	$h = -6 \rightarrow 8$
Absorption correction: None	$k = -9 \rightarrow 8$
7510 measured reflections	$l = -28 \rightarrow 34$
3094 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.048$	H-atom parameters constrained
$wR(F^2) = 0.127$	$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2 + 0.1253P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
3094 reflections	$\Delta\rho_{max} = 0.17$ e Å^{-3}
190 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.11303 (15)	0.36756 (17)	0.59259 (4)	0.0477 (3)
N1	−0.13352 (19)	0.2389 (2)	0.47654 (5)	0.0459 (4)
N2	0.25074 (18)	0.24104 (18)	0.52218 (5)	0.0379 (3)
C1	0.2995 (2)	0.3759 (2)	0.61786 (6)	0.0392 (4)
C2	0.4441 (2)	0.4866 (2)	0.59948 (6)	0.0447 (4)
H2	0.4210	0.5499	0.5695	0.054*
C3	0.6192 (2)	0.5003 (2)	0.62616 (6)	0.0435 (4)
H3	0.7168	0.5723	0.6138	0.052*
C4	0.6559 (2)	0.4077 (2)	0.67216 (6)	0.0371 (4)
C5	0.5053 (2)	0.3003 (2)	0.69082 (6)	0.0394 (4)
C6	0.3253 (2)	0.2858 (2)	0.66207 (6)	0.0412 (4)
H6	0.2253	0.2147	0.6735	0.049*
C7	0.8364 (2)	0.4201 (3)	0.70077 (6)	0.0483 (5)
H7	0.9372	0.4892	0.6888	0.058*
C8	0.8642 (3)	0.3322 (3)	0.74553 (7)	0.0618 (6)
H8	0.9839	0.3414	0.7638	0.074*
C9	0.7154 (3)	0.2285 (3)	0.76428 (7)	0.0694 (6)
H9	0.7355	0.1704	0.7953	0.083*

C10	0.5402 (3)	0.2116 (3)	0.73751 (7)	0.0593 (5)
H10	0.4424	0.1406	0.7502	0.071*
C11	0.0985 (2)	0.3003 (2)	0.54445 (6)	0.0375 (4)
C12	−0.0954 (2)	0.2999 (2)	0.52209 (6)	0.0439 (4)
H12	−0.1976	0.3445	0.5406	0.053*
C13	0.0233 (2)	0.1738 (2)	0.45104 (6)	0.0389 (4)
C14	−0.0076 (3)	0.1015 (3)	0.40208 (6)	0.0520 (5)
H14	−0.1333	0.1008	0.3867	0.062*
C15	0.1453 (3)	0.0325 (3)	0.37707 (7)	0.0561 (5)
H15	0.1237	−0.0157	0.3447	0.067*
C16	0.3351 (3)	0.0340 (2)	0.39983 (7)	0.0524 (5)
H16	0.4385	−0.0139	0.3824	0.063*
C17	0.3705 (2)	0.1044 (2)	0.44705 (6)	0.0430 (4)
H17	0.4977	0.1063	0.4615	0.052*
C18	0.2149 (2)	0.1739 (2)	0.47388 (5)	0.0348 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0342 (6)	0.0636 (9)	0.0449 (6)	0.0032 (5)	−0.0035 (5)	−0.0096 (6)
N1	0.0344 (8)	0.0508 (10)	0.0517 (8)	−0.0015 (6)	−0.0080 (6)	0.0037 (7)
N2	0.0336 (7)	0.0387 (8)	0.0409 (7)	−0.0003 (6)	−0.0048 (5)	0.0016 (6)
C1	0.0348 (9)	0.0424 (11)	0.0402 (9)	0.0010 (7)	−0.0013 (7)	−0.0076 (7)
C2	0.0497 (10)	0.0453 (11)	0.0389 (9)	−0.0025 (8)	−0.0017 (7)	0.0046 (8)
C3	0.0441 (9)	0.0424 (11)	0.0441 (9)	−0.0095 (8)	0.0033 (7)	0.0009 (8)
C4	0.0376 (8)	0.0339 (10)	0.0398 (8)	0.0010 (7)	0.0004 (6)	−0.0055 (7)
C5	0.0420 (9)	0.0356 (10)	0.0404 (9)	0.0010 (7)	0.0010 (7)	0.0008 (7)
C6	0.0392 (9)	0.0390 (11)	0.0457 (9)	−0.0056 (7)	0.0052 (7)	−0.0005 (8)
C7	0.0382 (9)	0.0534 (13)	0.0529 (10)	−0.0002 (8)	−0.0015 (7)	−0.0099 (9)
C8	0.0510 (12)	0.0723 (16)	0.0603 (12)	0.0077 (10)	−0.0177 (9)	−0.0017 (10)
C9	0.0681 (15)	0.0816 (17)	0.0571 (12)	0.0052 (12)	−0.0130 (10)	0.0210 (11)
C10	0.0594 (12)	0.0617 (15)	0.0566 (11)	−0.0039 (10)	−0.0004 (9)	0.0194 (10)
C11	0.0366 (9)	0.0351 (10)	0.0404 (8)	−0.0013 (7)	−0.0033 (7)	0.0026 (7)
C12	0.0332 (8)	0.0476 (11)	0.0506 (10)	0.0030 (8)	−0.0019 (7)	0.0007 (8)
C13	0.0387 (9)	0.0341 (10)	0.0431 (9)	−0.0050 (7)	−0.0058 (7)	0.0045 (7)
C14	0.0502 (11)	0.0557 (13)	0.0486 (10)	−0.0079 (9)	−0.0138 (8)	−0.0009 (9)
C15	0.0689 (13)	0.0558 (14)	0.0431 (10)	−0.0075 (10)	−0.0046 (9)	−0.0087 (9)
C16	0.0559 (11)	0.0509 (13)	0.0507 (10)	0.0038 (9)	0.0047 (8)	−0.0040 (9)
C17	0.0401 (9)	0.0415 (11)	0.0473 (9)	0.0018 (7)	−0.0013 (7)	0.0025 (8)
C18	0.0360 (8)	0.0295 (9)	0.0386 (8)	−0.0029 (7)	−0.0036 (6)	0.0060 (7)

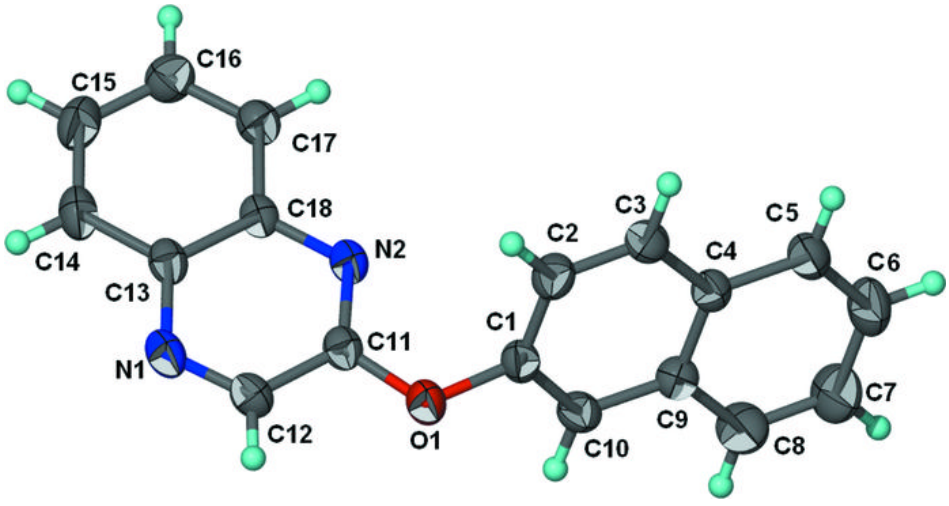
Geometric parameters (Å, °)

O1—C11	1.3622 (18)	C7—H7	0.9300
O1—C1	1.4073 (18)	C8—C9	1.391 (3)
N1—C12	1.297 (2)	C8—H8	0.9300
N1—C13	1.377 (2)	C9—C10	1.363 (3)
N2—C11	1.2928 (19)	C9—H9	0.9300
N2—C18	1.3778 (19)	C10—H10	0.9300

C1—C6	1.352 (2)	C11—C12	1.421 (2)
C1—C2	1.398 (2)	C12—H12	0.9300
C2—C3	1.359 (2)	C13—C14	1.405 (2)
C2—H2	0.9300	C13—C18	1.411 (2)
C3—C4	1.410 (2)	C14—C15	1.360 (3)
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.415 (2)	C15—C16	1.399 (2)
C4—C7	1.415 (2)	C15—H15	0.9300
C5—C10	1.410 (2)	C16—C17	1.361 (2)
C5—C6	1.414 (2)	C16—H16	0.9300
C6—H6	0.9300	C17—C18	1.401 (2)
C7—C8	1.357 (2)	C17—H17	0.9300
C11—O1—C1	118.73 (12)	C8—C9—H9	119.8
C12—N1—C13	116.62 (13)	C9—C10—C5	120.83 (19)
C11—N2—C18	115.58 (13)	C9—C10—H10	119.6
C6—C1—C2	122.30 (15)	C5—C10—H10	119.6
C6—C1—O1	117.50 (15)	N2—C11—O1	121.55 (13)
C2—C1—O1	119.95 (14)	N2—C11—C12	124.14 (15)
C3—C2—C1	118.92 (15)	O1—C11—C12	114.31 (14)
C3—C2—H2	120.5	N1—C12—C11	121.72 (15)
C1—C2—H2	120.5	N1—C12—H12	119.1
C2—C3—C4	121.39 (16)	C11—C12—H12	119.1
C2—C3—H3	119.3	N1—C13—C14	119.82 (15)
C4—C3—H3	119.3	N1—C13—C18	121.02 (14)
C3—C4—C5	118.72 (14)	C14—C13—C18	119.14 (15)
C3—C4—C7	122.55 (16)	C15—C14—C13	120.36 (16)
C5—C4—C7	118.72 (15)	C15—C14—H14	119.8
C10—C5—C4	118.70 (15)	C13—C14—H14	119.8
C10—C5—C6	122.33 (16)	C14—C15—C16	120.19 (16)
C4—C5—C6	118.97 (14)	C14—C15—H15	119.9
C1—C6—C5	119.65 (15)	C16—C15—H15	119.9
C1—C6—H6	120.2	C17—C16—C15	120.98 (17)
C5—C6—H6	120.2	C17—C16—H16	119.5
C8—C7—C4	120.72 (17)	C15—C16—H16	119.5
C8—C7—H7	119.6	C16—C17—C18	119.89 (16)
C4—C7—H7	119.6	C16—C17—H17	120.1
C7—C8—C9	120.65 (17)	C18—C17—H17	120.1
C7—C8—H8	119.7	N2—C18—C17	119.67 (14)
C9—C8—H8	119.7	N2—C18—C13	120.91 (14)
C10—C9—C8	120.38 (18)	C17—C18—C13	119.43 (14)
C10—C9—H9	119.8		
C11—O1—C1—C6	−119.60 (16)	C18—N2—C11—O1	178.93 (14)
C11—O1—C1—C2	65.9 (2)	C18—N2—C11—C12	−0.3 (2)
C6—C1—C2—C3	2.0 (3)	C1—O1—C11—N2	1.5 (2)
O1—C1—C2—C3	176.20 (15)	C1—O1—C11—C12	−179.20 (15)
C1—C2—C3—C4	−1.1 (3)	C13—N1—C12—C11	0.3 (2)
C2—C3—C4—C5	−0.7 (2)	N2—C11—C12—N1	−0.2 (3)
C2—C3—C4—C7	−179.77 (16)	O1—C11—C12—N1	−179.53 (15)

C3—C4—C5—C10	−178.29 (16)	C12—N1—C13—C14	178.37 (16)
C7—C4—C5—C10	0.8 (2)	C12—N1—C13—C18	0.1 (2)
C3—C4—C5—C6	1.7 (2)	N1—C13—C14—C15	−178.25 (17)
C7—C4—C5—C6	−179.25 (15)	C18—C13—C14—C15	0.0 (3)
C2—C1—C6—C5	−1.1 (3)	C13—C14—C15—C16	−0.4 (3)
O1—C1—C6—C5	−175.37 (14)	C14—C15—C16—C17	−0.2 (3)
C10—C5—C6—C1	179.15 (16)	C15—C16—C17—C18	1.1 (3)
C4—C5—C6—C1	−0.8 (2)	C11—N2—C18—C17	−179.07 (14)
C3—C4—C7—C8	178.35 (17)	C11—N2—C18—C13	0.8 (2)
C5—C4—C7—C8	−0.7 (3)	C16—C17—C18—N2	178.38 (15)
C4—C7—C8—C9	−0.2 (3)	C16—C17—C18—C13	−1.5 (2)
C7—C8—C9—C10	1.0 (3)	N1—C13—C18—N2	−0.7 (2)
C8—C9—C10—C5	−0.9 (3)	C14—C13—C18—N2	−178.94 (15)
C4—C5—C10—C9	0.0 (3)	N1—C13—C18—C17	179.13 (15)
C6—C5—C10—C9	−179.97 (18)	C14—C13—C18—C17	0.9 (2)

Fig. 1


C16
C15
C17
C18
N2
C14
C13
C11
N1
C12
O1
C1
C2
C3
C4
C5
C6
C7
C8
C9
C10